tumor with heterogeneous vascular distribution, and various dextrans were chosen as the drug carrier to study the impact of the sizes of tumor and necrotic region, and vascular surface area per unit tumor volume (*S/V*) on the average accumulative concentration. The results showed that: 1) large nanoparticles produced a high accumulative concentration in the well-vascular region, but low dose in the necrotic region; 2) small nanoparticles can penetrate into the necrotic region; however, its accumulative concentration was low and was more toxic to the normal tissue; 3) the influence of the tumor size on the average accumulative concentration was much more pronounced for small nanoparticles, while the effect of *S/V* was relatively more significant when employing large nanoparticles. The results indicated that the effectiveness of the anti-tumor drug delivery was determined by the interplay of the vascular density and nanoparticle size, and the proposed model can serve as a useful guide in tailoring tumor treatments.

3113-Pos Board B805

Application of Cup Shaped Superparamagnetic Hemispheres for Size Selective Cell Purification

Hyonchol Kim[1], Hideyuki Terazono[1,2], Hiroyuki Takei[1,3], Kenji Yasuda[1,2].
[1]Kanagawa Academy of Science and Technology, Kanagawa, Japan, [2]Tokyo Medical and Dental University, Tokyo, Japan, [3]Toyo University, Gunma, Japan.

Purification of specific target cells from complex cell ensemble is essential step in life science studies. Magnetic cell sorting (MACS) is one famous method to purify target cells depending on the specific recognition of ligands immobilized on the magnetic particles against the target cell. For the improvement of this method, one useful way is target cell recognition with not only ligand specificity but also other physical parameters. Here we report another way for the recognition and purification of target cells depending on their sizes using a new type magnetic particle.

The particle was fabricated as follows. Polystyrene spheres were used as templates, coated with magnetic elements (Ni was used in this study) by thermal evaporation, and burned to remove polystyrene templates. Then, cup-shaped hemispheres composed of the evaporated elements were obtained. We succeeded for the fabrication of superparamagnetic hemispheres (referred as "Mag cups", hereafter) by controlling the thickness of magnetic element layers strictly. Target cells were size-selectively captured into the inner cavity of the Mag cups, and easily collected with an application of the magnetic field. We found that the cells can be only collected using larger cups than target cell diameter, indicated that fabricated Mag cups can be used for size-selective cell purifications.

3114-Pos Board B806

Molecular Dynamics Study of Self-Assembled Lipid Nano-Particles for Drug Delivery

Dmitri Rozmanov, Peter Tieleman.
University of Calgary, Calgary, AB, Canada.

One of the main methods for delivery of therapeutic siRNA to targeted cells is the systematic delivery inside lipid nano-particles (LNP). Detailed understanding of the internal structure of such LNPs is essential for designing more efficient drug delivery systems in terms of the particle size, level of siRNA encapsulation, protection of siRNA against degradation, and targeting and release of siRNA. Our current understanding of the internal structure of such nano-particles is still limited [J. Phys. Chem. C, 2012, 116, 18440].

In this work the structure of nano-particles relevant for drug delivery is studied by molecular dynamics simulations in the frame work of the coarse-grained MARTINI force field. Spontaneous self-assembly was initiated from various initial configurations with different distribution of the components and was followed in time to identify the most stable form of the particle. The common structural motives of assembled nano-particles are used to propose a plausible structure for real drug delivery LNPs. The LNPs studied in this work are composed mainly of an ionizable cationic lipid, a structural phospholipid, and cholesterol. The simulations were done both in the presence of a therapeutic polynucleotide and without it. Various structural properties of the emerging nano-particles are analyzed along the simulation trajectory to evaluate the convergence of the observed structures. Particular attention is paid to the water content of the nascent LNPs as well as to the size distribution of the cavities containing the internal water.

3115-Pos Board B807

Molecular Theory of Protein Sorption on Weak Polyelectrolyte Gel-Modified Charged Surface

Claudio F. Narambuena, Gabriel Longo, Igal Szleifer.
Northwestern University, Evanston, IL, USA.

We developed a detailed molecular theory to determine protein adsorption on a charged surface as a function of the pH, salt concentration, protein concentration and surface charge density, as well as the modification of the surface by the attachment of a weak polyelectrolyte gel film. The approach includes specific molecular details of the proteins, their translational and rotational degrees of freedom as well as the acid-base equilibrium of the titratable amino acids. We also include the conformational degrees of freedom and acid-base equilibrium of the polymeric gel, the solution entropic contributions, and electrostatic and excluded-volume interactions. The experimental titration curve of lysozyme and the isoelectric point (IP) in solution are reproduced successfully. In low salt conditions, lysozyme adsorption profiles as a function of pH on a non-modified surface are broad and have a maximum value at a pH lower than the isoelectric point of the protein. When the salt concentration is increased, maximum adsorption occurs at evenlower pH values. The level of protein adsorption on a gel-modified surface is two orders of magnitude greater than on a non-modified surface, and has a narrower maximum close to the IP at low salt concentration. The molecular theory may explain the excellent properties of such modified surfaces for chromatographic separation of proteins as well as help to design new chromatographic systems. Moreover, the theory provides with a fundamental understanding of the competition between the different contribution that determine the adsorption behavior.

3116-Pos Board B808

Antibody-Based Magnetic Nanoparticle Immunoassay for Quantification of Salivary Beta-Amyloid Peptides

Chang-Beom Kim, Ki-Bong Song.
Consilience technology research section, Electronics and Telecommunications Research Institute, Daejeon, Korea.

Alzheimer's disease (AD) is a neurodegenerative disorder that leads to a decline in cognitive and intellectual ability and irreversible mental deterioration. Based on the multidisciplinary AD researches, the most universally accepted hypotheses on AD pathogenesis are the intracerebral aggregate formation of beta-amyloid (Aβ) peptides. According to medical paradigmatic transition from medical treatment to early diagnostic prevention, scientists have considered physiological body fluid as biomarker medium in which the promising AD biomarkers could be verified. Recently, use of saliva has been considered as one of the diagnostic fluids over the past decade with meaningful diagnostic potential.We utilized saliva as a biomarker medium to correlate the salivary Aβ levels to AD pathological aspects, especially to the MCI group among AD patients to verify our detecting system to be sensitive for early diagnostic tool. The identification of the salivary AD biomarkers using a facile microarraying method would motivate this study with the assistance of magnetically assembled antibody-conjugated nanoparticles and PMT as optical detector. This simple magnetoimmunoassay system measures the photo intensity generated by fluorescence, enables the quantification of the Aβ peptides from AD salivary samples, and consequently classifies the salivary Aβ levels into AD pathological aspects. This method demonstrates a facile approach enabling to simply detect salivary Aβ peptides at a concentration as low as ~20 pg/ml. It is expected that our simple magnetoimmunoassay system may have a potential as a detector for low-level Aβ peptides with weak fluorescence emission.

3117-Pos Board B809

Synthesis of Graphene-Based Nanomaterials for Biosensing

Yong Ju Yun, Ki-bong Song.
Electronics and Telecommunications Research Institute(ETRI), Daejeon, Korea, Republic of.

Graphene-based hybrid composites have offered significantly improved performance for various applications including optoelectronic devices, electrocatalysts, lithium ion batteries and supercapacitors due to their unique properties such as good optical and electrical property and high specific surface area. Among them, the graphene/gold nanoparticle composites have been attractive attention in recent years because of their new optical, electrical, catalytic properties. Various gold nanomaterials, such as gold nanoparticles, gold nanorods, have been successfully assembled onto GO nanosheet by the chemical reduction of gold ions and the adsorption of gold nanomaterials. However, the synthesis of the graphene/gold hybrid contains a somewhat tiresome process. Additional heat treatments or complicated surface chemical treatment of the gold nanoparticles are needed to achieve the composites. Herein, we introduce a facile and simple method for synthesizing graphene oxide encapsulated gold nanoparticles (GOGNPs) based on electrostatic interaction between negatively charged graphene oxide and positively charged beta amyloid protein coated gold nanoparticles. The morphology and structure of the GOGNPs were confirmed by transmittance electron microscopy (TEM) and scanning electron microscopy (SEM).